UCRL-WEB-201522

LINMath User Guide

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Preface

Function: LINMath (Livermore Interactive Numerical Mathematics utility) is a customized world-wide web site for LLNL users that provides approximately the same subroutine-finding, advice-giving, and source-retrieval features as did the former NMG utility. LINMath relies on the widely used GAMS (URL: http://www.llnl.gov/LCdocs/gams) scheme for classifying mathematical software. LINMath directly covers LC-supplied Fortran and C mathematical libraries, with links to information on externally supplied libraries.

Availability: LINMath is a WWW site on LC's open network, with access limited to machines within the LLNL domain(s). A comparable SCF LINMath site is available on LC's secure network (with passworded access and its own URL).

Consultant: For help contact the LC customer service and support hotline at 925-422-4531 (open e-mail: lc-hotline@llnl.gov, secure e-mail: lc-hotline@pop.llnl.gov).

This manual was adapted from LLNL technical report UCRL-MA-125006, Part 1, developed and written by Frederick N. Fritsch and Robert P. Dickinson, Jr.

Printing: The print file for this document can be found at:

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on the OCF: http://www.llnl.gov/LCdocs/nmg1/nmg1.pdf
on the SCF: https://lc.llnl.gov/LCdocs/nmg1/nmg1_scf.pdf
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1. NMG-LINMath Background

LC once had a group of computational mathematicians (the Mathematical Software Service), who designed and deployed an interactive utility to assist users in selecting appropriate mathematical software and in delivering documentation and source code for the routines the user selected. This utility was called the Numerical Mathematics Guide, NMG. It ran in several environments, but primarily on LC's secure CRAY J90 computers, which were retired from public production in March, 2000. When the CRAYs retired, so did NMG.

NMG was command driven, and its three most important commands were:

menu	Provided access to a complete menu of all user-level routines in the LC-supplied mathematical and statistical libraries.
advice	Offered advice on routine selection, using a special Advisor program.
fetch	Delivered online documentation and source code (when available) for individual routines selected using the other commands.

When NMG's developers created a pair of web sites (called LINMath, (page 5) one open and one secure) to provide many of the same services as NMG, these three commands shaped their design. Thus NMG's intellectual content and user-service functions live on in the various levels of LINMath, delivered now by World-Wide Web browsers rather than by executing overt commands. The remainder of this document tells how to use LINMath today to get the help with computational mathematics formerly provided by NMG.

2. LINMath (Web-based NMG)

2.1. Role

LINMath (Livermore Interactive Numerical Mathematics utility) is a pair of customized world-wide web sites that delivers advice on and descriptions of mathematical library subroutines, as well as the subroutine source files themselves. The LINMath web site uses the standard GAMS (URL: http://www.llnl.gov/LCdocs/gams) (Guide to Available Mathematical Software) hierarchical system for organizing math routines to structure its menu tree. In fact, you can regard LINMath as an LLNL-oriented, advice-enriched version of the original GAMS web site (URL: http://gams.nist.gov) created by the U.S. National Institute for Standards and Technology (NIST).

Users of the former NMG utility on LC's secure Cray computers will recognize LINMath as a web-based version of NMG. Of course, LINMath relies on interactive hypertext links and other common web browser (client) features, rather than on commands typed in response to prompts, to navigate its structure and ultimately to deliver appropriate mathematical software. Partly for this reason, LINMath combines into a single tree three features that were available as separate NMG commands:

- Menu (browsing by hierarchical topics, using the GAMS subject categories).
- Advice (comparative and strategic tips on numerical methods).
- Fetch (downloading of actual math subroutines, with comment documentation, to compile and use).

For a broad comparison and survey of the mathematical libraries and tools (such as MATHEMATICA) available on LC production machines, consult LC's Mathematical Software Overview. (URL: http://www.llnl.gov/LCdocs/math) (Some preinstalled libraries discussed there, such as FFTW and SPRNG, are not delivered using LINMath.)

2.2. Coverage

The LINMath web site covers four local (LC noncommercial) math libraries, on which it can deliver source files as well as advice:

- SLATEC (over 900 user-callable routines)--a large and diverse library developed by a multilaboratory collaboration. Detailed manuals (URL: http://www.llnl.gov/LCdocs/slatec1) are available online.
- MSSL (about 100 routines)--a more specialized library assembled and thoroughly tested at LLNL (but not preinstalled).
- MSSL3 (about 300 routines)--also assembled at LLNL but less thoroughly tested and screened; many are very useful but originated elsewhere. (At LC, use the service routines I1MACH and R1MACH from MSSL3 rather than from SLATEC for more accurate and appropriate results. See the "Largest and Smallest Numbers" section of LC's Mathematical Software Overview (URL: http://www.llnl.gov/LCdocs/math) for details.)
- PMATH (68 routines)--a more specific, portable version of the older but much-used MATHLIB library. A PMATH manual (URL: http://www.llnl.gov/LCdocs/pmath) is available online.

Note that the versions of SLATEC and PMATH subroutines provided by LINMath are often more recently improved and debugged, while those installed on each machine as compiled object code have remained unaltered since 1996. So LINMath is the preferred source for all the libraries that it covers, even where they are available otherwise.

LINMath also provides advice on and numerous pointers to (but NOT directly the source files for) many external collections of math software, most available indirectly through the Internet. Among these referenced external software collections are:

- Netlib--a large collection maintained by Oak Ridge National Laboratory, UTK, and the former Bell Labs.
- GAMS/HotGAMS--a large categorized collection managed by the National Institute for Standards and Technology.
- HPC-Netlib--a large collection maintained by the National High Performance Computing and Communication Software Exchange (NHSE).
- ACM Collected Algorithms--a collection of algorithms published by the Association for Computing Machinery.

2.3. User Instructions

To use the open (OCF) LINMath web site, execute any standard WWW browser (client) and request the open-network URL

`http://www-r.llnl.gov/icc/linmath`

As the URL implies (www-r), the LINMath server automatically restricts access to only those clients running on machines within the LLNL domain(s) (or with equivalent virtual connections). No special login name or password is required for access from domain-eligible machines. The restrictions are needed because LINMath can deliver actual math-library source code to its users, not just descriptions of when to use that code.

A comparable LINMath site, offering the same question-answering and source-delivery services, is also available to SCF users at this secure-network URL (requires DCE password):

`https://lc.llnl.gov/linmath/`

[WARNING: note both the 's' in https and the final slash (/) character in this URL. You must include BOTH to successfully reach the SCF version of LINMath. The SCF URL was changed in August, 2002.]

The LINMath web site uses few graphics and no frames, so it runs successfully (and with stunning speed) for text-only web clients (such as LYNX), which disabled users may find especially convenient. The site does not include any overt navigational links (e.g., back one level, parent class, top of tree), however. So you should rely on your browser's own BACK and GO features to climb back up any menu branch that you have descended.

Because the LINMath site is divided among many separate files, you cannot display (or print) the entire GAMS classification scheme from the site itself. If a comprehensive and comparative overview of the entire GAMS scheme would help you with LINMath planning and subroutine decisions, consult the separate GAMS online document (URL: http://www.llnl.gov/LCdocs/gams). This document contains NIST's complete Guide to Available Mathematical Software. You can easily display or print (with File/Print Frame) the full set of subject headings for any GAMS subject category using your WWW client. Or you can print the entire 28-page GAMS document for reference by getting its PostScript file from either the open or secure LC anonymous FTP server using the printing directions in the Documentation Guide (URL: http://www.llnl.gov/LCdocs/docguide) (or in its first section).

2.4. Comparison with NMG Features

LINMath provides three basic services (browsing math categories, getting advice on best routine choices, and downloading the actual code). These services are spread (in order) from top to bottom among the web-site levels as shown in this diagram (and as explained below it):

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Service     Levels in LINMath Tree
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Menu        Top three levels:
[browse]    1. Highest-level GAMS categories listed
               2. Broad areas of math (for each category)
                  3. Specific numerical problems (for each area)

Advice      Middle three levels:
            4. Generally relevant numerical methods, tips
               5. Specific computational techniques compared
                  6. Promising individual routines described

Fetch       Bottom level:
[download]  7. Actual text of routine prolog followed by
               commented source code
```

TOP THREE LEVELS (MENU).
The top level ("home page") of the LINMath web site briefly introduces the role and scope of this math-library user aid. It then lists the (16) highest-level GAMS subject categories of math routines, each linked to the appropriate list of subcategories below it. At this level, LINMath closely resembles the MENU mode of the former NMG tool (except that MENU mode showed several layers of GAMS categories at once). In LINMath, you must select a GAMS category to see its children, then choose one subcategory to see a third layer of subject-category detail.

MID THREE LEVELS (ADVICE).
As you follow links down to the middle layers of the GAMS subject hierarchy, LINMath starts to mimic the ADVICE mode of the former NMG tool. For each middle layer, it offers

- General, strategic advice for making the best use of routines of the type you have chosen, or for good numerical solutions to the type of problem you are exploring, and
- A list of recommended math subroutines, grouped by library, and
- A list of relevant libraries showing the number of appropriate routines in each one (with links to the subroutine details).

LOWEST LEVEL (FETCH).
At the bottom of the LINMath menu tree the site displays (in "preformatted" plain text) the descriptive prolog for the specific math subroutine(s) that you have chosen, followed by the actual code for the routine(s). There are no more prompts or links at this bottom level (about file delivery), but you can regard it as LINMath's approximation to the old NMG FETCH mode. By using the File/Save As (or equivalent) menu items on your web client, you can deposit the displayed subroutine code into a file of your choice on the machine where your web client runs.

There are also no upward links to previous GAMS layers or to the top of the LINMath tree. But you can use your web client's BACK and GO buttons to climb back up the tree or jump to the top to start down a different branch. This is not trivial, however, because all branches have the same label ("LINMath menu") rather than their GAMS subject code or descriptor. (To see the whole GAMS classification scheme spelled out in hierarchical format as a planning or retrieval aid when you use LINMath, consult LC's GAMS document (URL: http://www.llnl.gov/LCdocs/gams), either online or in print.)

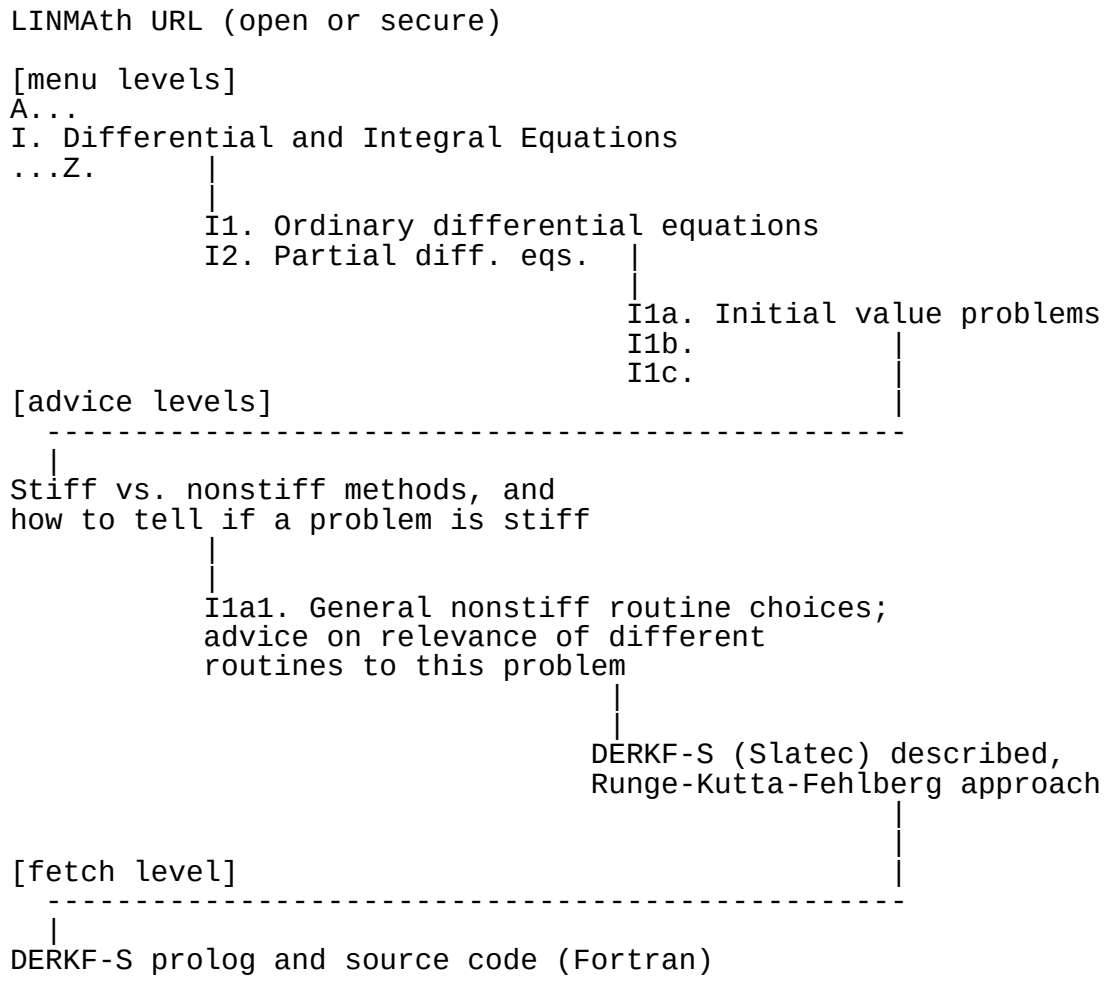
2.5. Example

[1]

GOAL: To get help in solving a (kind of) initial-value problem numerically, using locally available math routines.

STRATEGY: (1) Execute your web client (browser) and go to the LINMath URL.
(2) Start at the top of the LINMath site and work down the layers to locate this kind of problem (top "menu" levels), then read relevant tips and comparisons of methods and routines (middle "advice" levels), then pick a specific library routine and check its prolog and source code (bottom "fetch" level).
(3) Use your browser's File/Save As (or equivalent) menu choice to deposit the code you want on the machine where your browser runs.

[Diagram of this strategy by web-site level follows:]


LINMAth URL (open or secure)
[menu levels]
A...
I. Differential and Integral Equations
...Z.
I1. Ordinary differential equations
I2. Partial diff. eqs.
I1a. Initial value problems
I1b.
I1c.
[advice levels]
Stiff vs. nonstiff methods, and
how to tell if a problem is stiff
I1a1. General nonstiff routine choices;
advice on relevance of different
routines to this problem
DERKF-S (Slatec) described,
Runge-Kutta-Fehlberg approach
[fetch level]
DERKF-S prolog and source code (Fortran)

Disclaimer

Keyword Index

To see an alphabetical list of keywords for this document, consult the next section (page 14).

Alphabetical List of Keywords

Keyword	Description
a	Alphabetical keyword list.
availability	Where LINMath is available.
date	Latest revision date for this document.
entire	This entire document.
function	Purpose of this software.
index	List of keywords in order of occurrence.
linmath	Web-based NMG-like math-help site.
linmath-coverage	Local and external libraries covered.
linmath-example	Sample LINMath session diagramed.
linmath-features	LINMath's 3 functions diagramed, compared.
linmath-role	LINMath's purpose and basic functions.
linmath-usage	LINMath's URL, restrictions, tips.
nmg-background	Numerical Math Guide, forerunner to LINMath.
revisions	Revision history of this document.
title	Title of this document.
web-math-access	Web-based NMG-like math-help site.
who	Who to contact for help.

Date and Revisions

Revision Date	Keyword Affected	Description of Change
04Sep02	linmath-usage	New URL for SCF LINMath.
11Jun02	linmath-role	Cross ref to Math Overview added.
	linmath-coverage	MSSL3 vs SLATEC warning added.
28May02	nmg-background	Faulty link activated.
04Feb02	linmath-usage	New URL for OCF LINMath.
	linmath-coverage	Newest SLATEC, PMATH routines in LIMath.
19Jul00	nmg-background	SCF LINMath now active.
	linmath-usage	New SCF LINMath URL, warnings.
20Mar00	linmath	Diagrams, usage details added.
	index	Most NMG terms deleted.
	nmg-background	NMG details removed, obsolete.
19Aug99	linmath	New URL, details revised.
	availability	SCF LINMath version noted.
21Jul98	linmath	New web interface explained.
	index	New keywords for new sections.
	availability	NMG on J90s only, LINMath added.
14Jul97	entire	"LC-supported" became "LC-supplied" in all sections.
	availability	Some machines deleted.
	who	Original NMG authors noted.
16Jul96	entire	First edition of NMG user manual.

TRG (04Sep02)

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TRG (04Sep02) Contact on the OCF: lc-hotline@llnl.gov, on the SCF: lc-hotline@pop.llnl.gov